

# 2,6-Pyridinedicarboxylic acid, dodecyl phenethyl ester

**Inchi:** InChI=1S/C27H37NO4/c1-2-3-4-5-6-7-8-9-10-14-21-31-26(29)24-18-15-19-25(28-24)27(30)26  
**InchiKey:** PZOXBIJASZILU-UHFFFAOYSA-N  
**Formula:** C27H37NO4  
**SMILES:** CCCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1  
**Mol. weight [g/mol]:** 439.59

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.36		Crippen Method
logp	6.559		Crippen Method
mcvol	368.630	ml/mol	McGowan Method
rinpola	3244.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369230&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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